

ABSTRACT OF THE DISCLOSURE

Methods and systems for drug discovery and development are disclosed. Methods and system consistent with the present invention discover drugs. One or more databases comprising chemical and biological interaction data and one or more computer-based data analysis programs may be used to identify compounds that have desired activity at two or more molecular targets that are associated with a disease state for which the drug discovery and development are directed. In addition, one or more databases comprising chemical and biological interaction data and one or more computer-based data analysis programs may be used to identify compounds that (a) have desired activity at one or more molecular targets that are associated with a disease state for which the drug discovery and development are directed and (b) do not have activity or have substantially reduced activity that is undesired at one or more molecular targets that are associated with possible side effects, toxicity, adverse ADME properties, or other properties not intended to be manifested by compounds being developed to treat the disease state associated with the drug discovery.

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